



Compound : Table

Field Name	Data Type	Description
Compound ID	Text	
Compound	Text	
CAS Number	Text	
Formular	Text	
Log P (pH)	Text	
Hammet Sigma	Text	
Other Parameters	Text	
Solubility	Text	
Structure	OLE Object	
Smile Codes	Text	
Rotatable Bonds	Text	
Known Toxicology	Text	
Originator	Text	
Vendor	Text	
Catalog Number	Text	
Molecular Weight	Text	
Patent	Text	
Literature	Hyperlink	
Comments	Hyperlink	
	Memo	

Field Properties

General

Lookup

Format
Caption
Default Value
Validation Rule
Validation Text
Required
Allow Zero Length

A field name can be up to 64 characters long, including spaces. Press F1 for help on field names.

Validation Text

Required

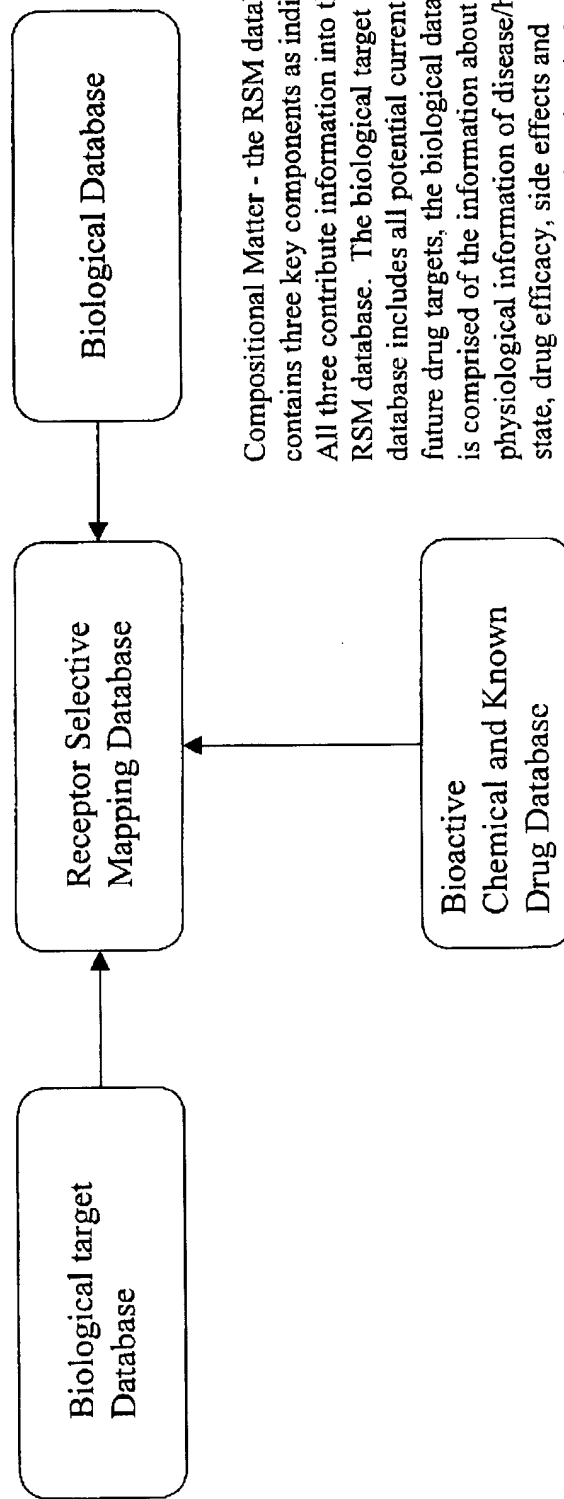
Allow Zero Length

No

No

Figure 1C

Three-component Database For Drug Discovery/Development



Compositional Matter - the RSM database contains three key components as indicated. All three contribute information into the RSM database. The biological target database includes all potential current and future drug targets, the biological database is comprised of the information about all physiological information of disease/healthy state, drug efficacy, side effects and toxicology. The bioactive chemical and known drug database contains chemicals that are known to be active against certain biological targets; useful in treating diseases. The chemical database also includes natural products in the form of biomass, extracts, or compounds that are not entirely from chemical synthetic origin.

Chart 2

FIG. 1D

to: 0

Look at: 0

X Selection 1 - 247

CA NH3+	1	XAQITGRPEW	IWLALGTALM	GLGTLYFLVK	GMGVSDPDPAK	KFYAITTLVP	AIAFTNYLSM	LLGYGLTMVP	FGGEQNPIYW
elix									
elix									
neet									
neet									
	81	ARYADWLETT	PLLLLDLALL	VDADQGTILA	LVGADGIMIG	TGLVGALTKV	YSYRFVWVAI	STAAMLYILY	VLFFGFTSKA
elix									
elix									
elix	161	ESMRPEVAST	FKVLRNVTWV	LWSAYPVVWL	IGSEGAGIYP	INIELLIFMV	LDVSAKVGFG	LILLRSRAIF	GEAEAPEPSA
elix									
elix									
RET, 301)	241	DGAAATS							

Figure 2A



toxicology : Table

Field Name	Data Type	Description
ID	AutoNumber	
LD50	Text	
Animal Models	Text	
Human Toxicity data Base1	Hyperlink	
Human Toxicity data Base2	Hyperlink	
Human Toxicity data Base3	Hyperlink	
MSDS	Hyperlink	
Target Organ (animals)	Text	
Target Organs (Human)	Text	
Teratogenicity	Text	
Mutagenicity	Text	
Reproductive Toxicity	Text	
Metabolites	Text	
Apoptosis	Text	
Necrosis	Text	
In vitro toxicity profile 20	Text	

Field Properties

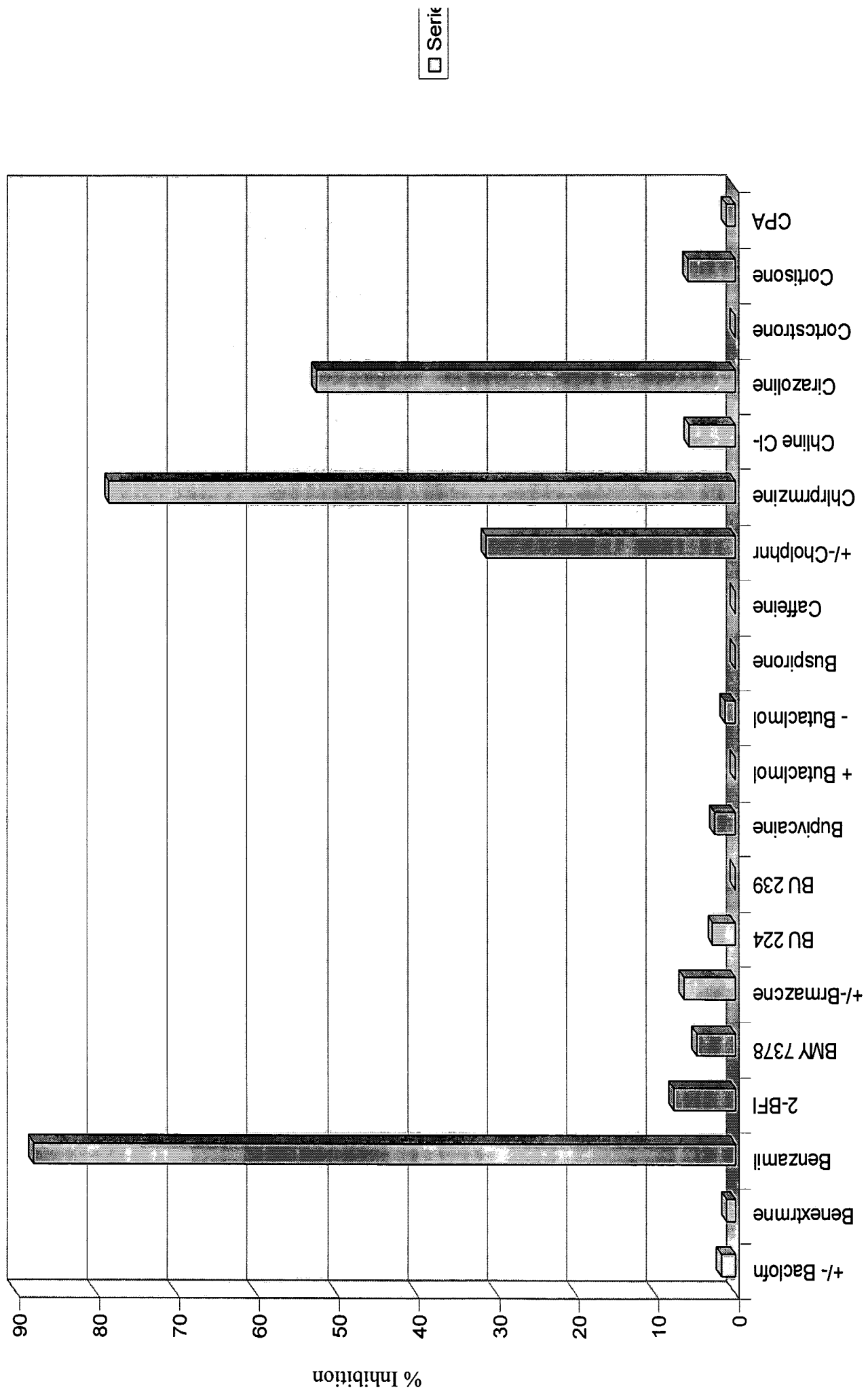
General	Lookup
Field Size	50
Format	
Input Mask	
Caption	
Default Value	
Validation Rule	
Validation Text	
Required	No
Allow Zero Length	No
Indexed	No

The field description is optional. It helps you describe the field and is also displayed in the status bar when you select this field on a form. Press F1 for help on descriptions.

Figure 3A

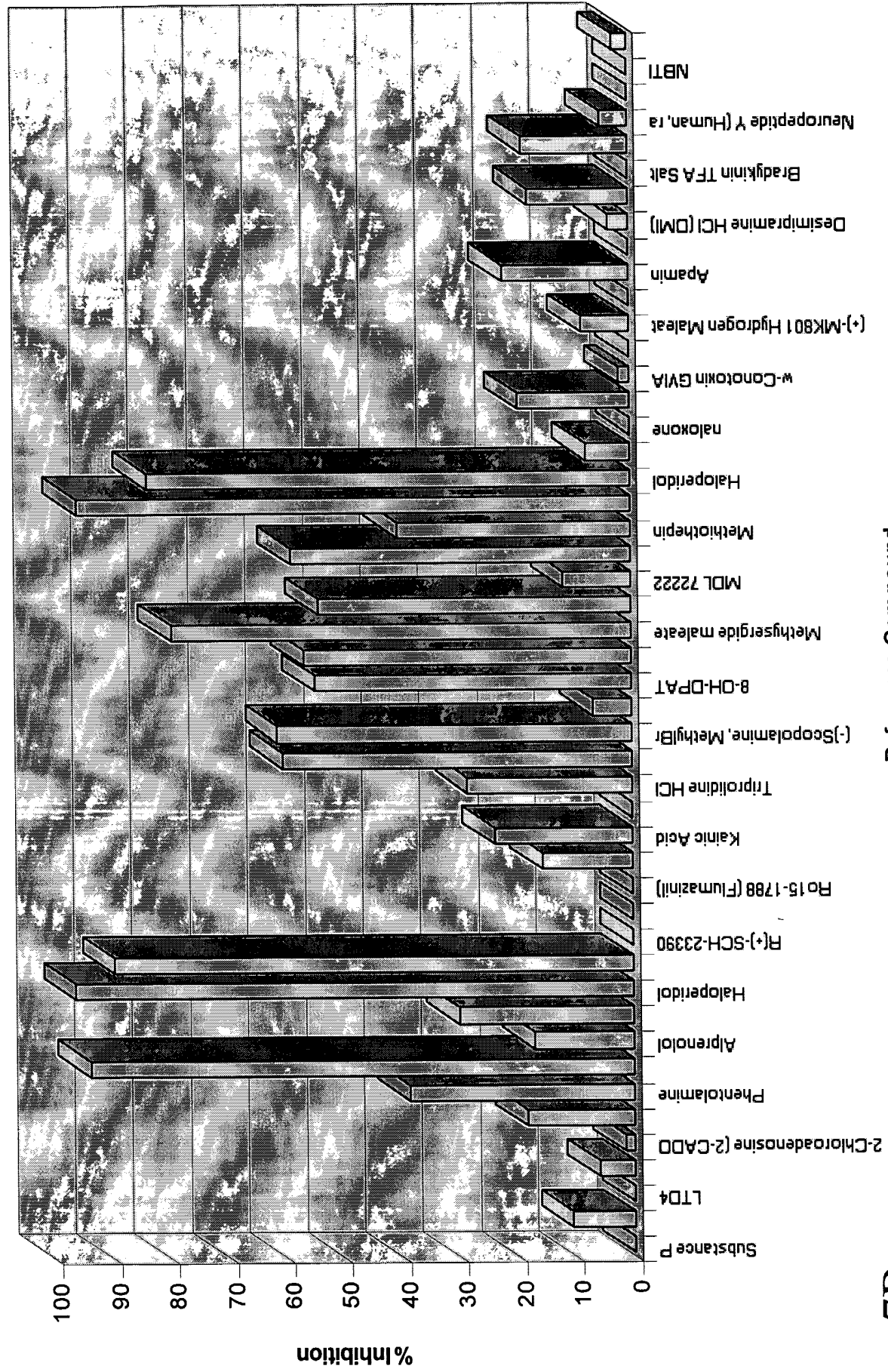
Figure 7A

Chemical profile - 5HT3



Serotonin, 5HT₄

Chemical Profile

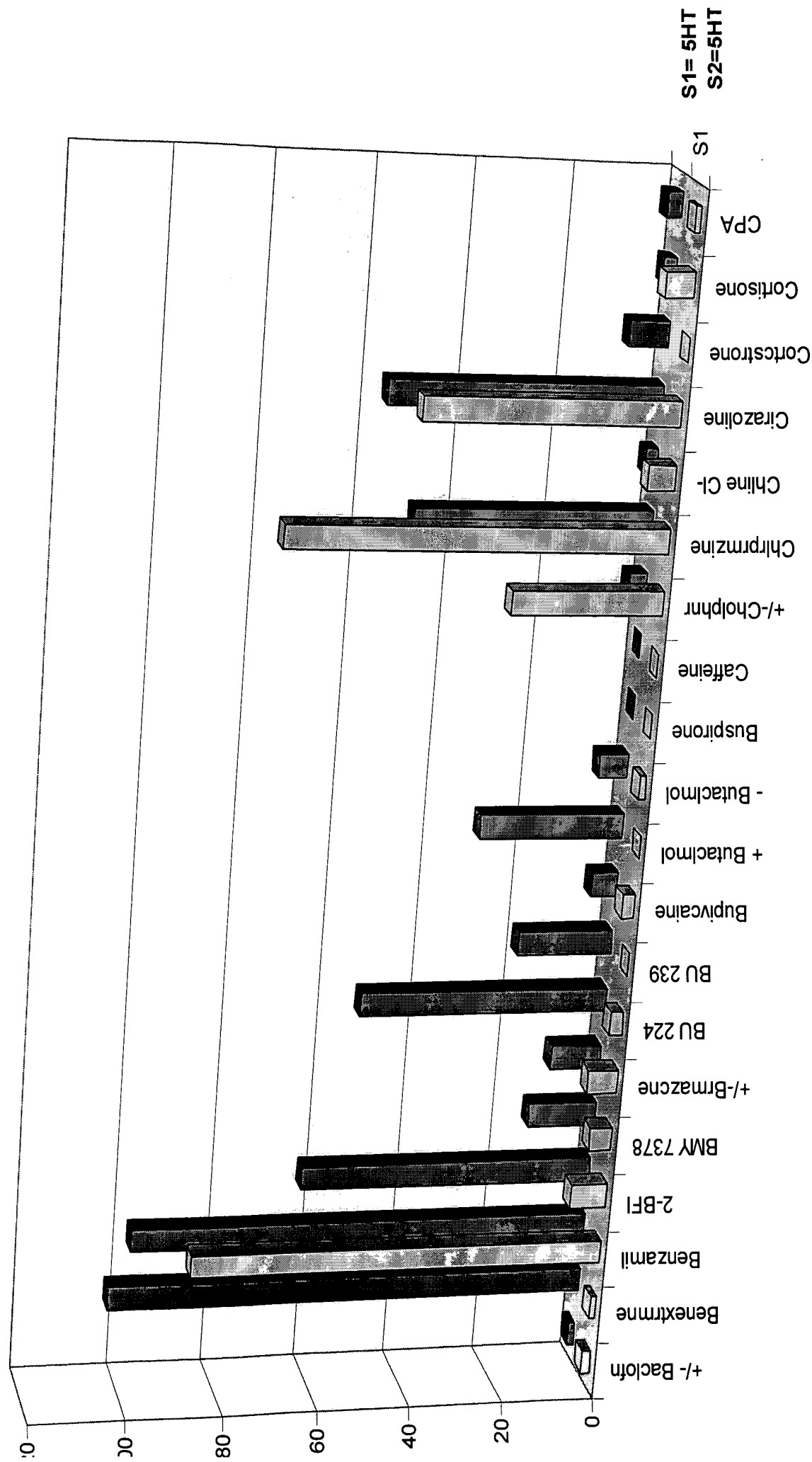


Reference Compound

Figure 7B

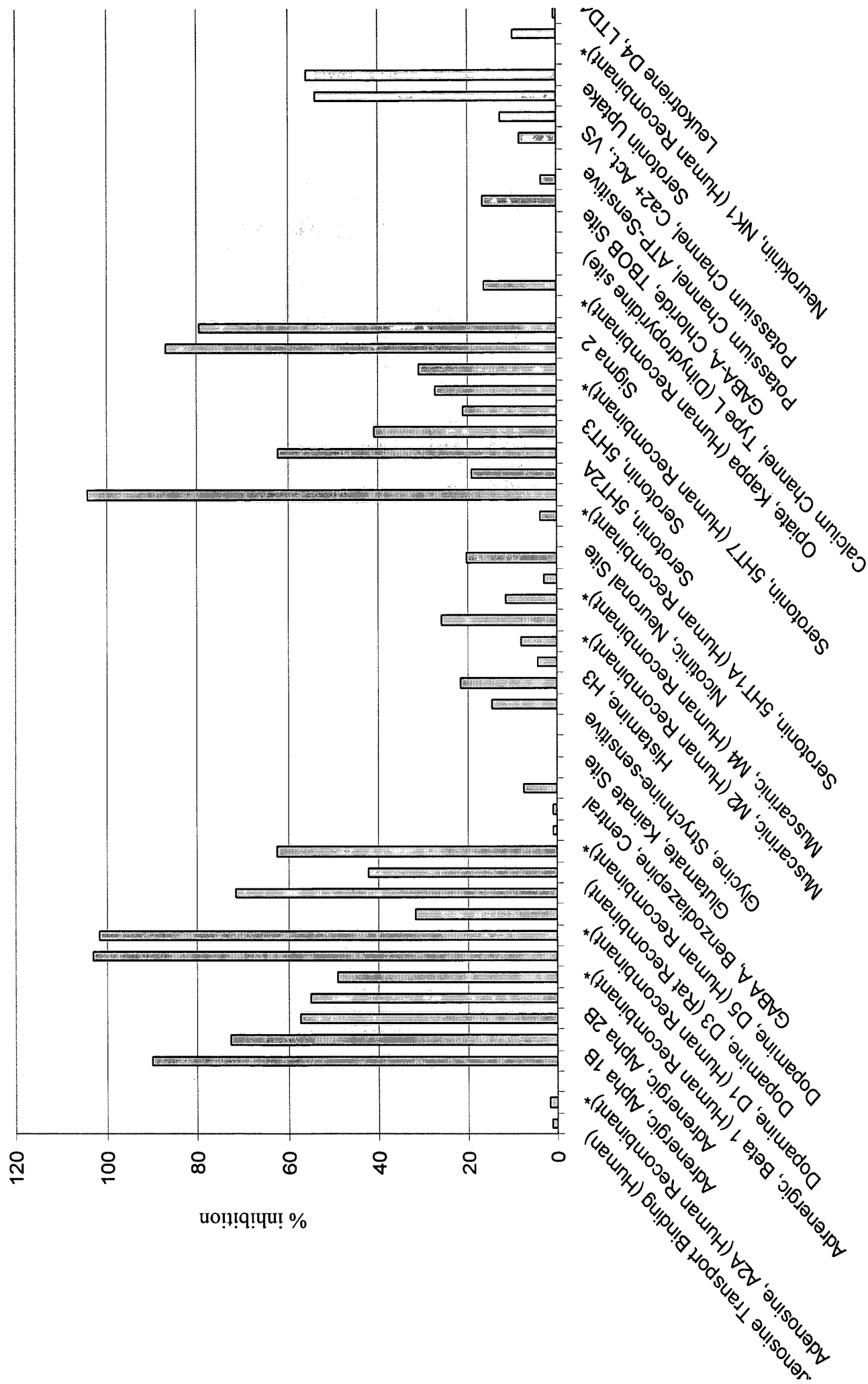
Chemical Profiles

5HT3 vs 5HT4



Reference Compounds

Figure 7C

[illegible]



Series 1=Albuterol
Series 2=Alprenolol

